Water

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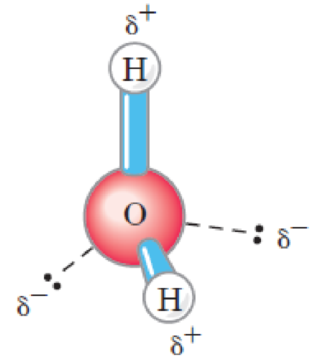
Water

- The water molecule and its ionization products, H and OH, profoundly influence the structure, self-assembly, and properties of all cellular components, including proteins, nucleic acids, and lipids.
- Hydrogen bonds between water molecules provide the cohesive forces that make water a liquid at room temperature and that favor the extreme ordering of molecules that is typical of crystalline water (ice).
- Polar biomolecules dissolve readily in water because they can replace water-water interactions with more energetically favorable water-solute interactions.
- In contrast, nonpolar biomolecules interfere with water-water interactions but are unable to form water-solute interactions—consequently, nonpolar molecules are poorly soluble in water.

Hydrogen Bonding Gives Water Its Unusual Properties

- Water has a higher melting point, boiling point, and heat of vaporization than most other common solvents.
- These unusual properties are a consequence of attractions between adjacent water molecules that give liquid water great internal cohesion.
- Each hydrogen atom of a water molecule shares an electron pair with the central oxygen atom.
- The geometry of the molecule is dictated by the shapes of the outer electron orbitals of the oxygen atom.
- An oxygen atom has a total of 8 electrons distributed in two energy levels, written as $\mathbf{1s^2\ 2s^2\ 2p^4}$.
- The "outer electron orbital" refers specifically to the second energy level (n=2), which acts as oxygen's valence shell.
- **The 2s Orbital:** This is a single, spherical orbital. It holds **2 paired electrons** spinning in opposite directions.
- **The 2p Orbitals:** This subshell contains three dumbbell-shaped orbitals ($2p_x$), ($2p_y$), and ($2p_z$) pointing in different directions. Together, they hold **4 electrons**.

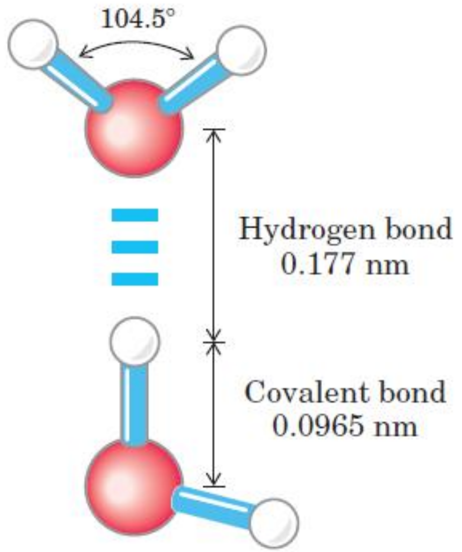
How the 2p Electrons are Arranged (Hund's Rule)



- Electrons naturally separate before they pair up to minimize repulsion. In the 2p subshell, the 4 electrons are distributed like this:
- **First orbital ($2p_x$):** Holds **2 paired electrons**
- **Second orbital ($2p_y$):** Holds **1 unpaired electron**
- **Third orbital ($2p_z$):** Holds **1 unpaired electron**
- Because oxygen has **2 unpaired electrons** in its outer shell, it eagerly seeks 2 more electrons from other atoms to fill its valence shell and become stable.
- This is why oxygen typically forms two chemical bonds, such as bonding with two hydrogen atoms to create water (H_2O).
- Oxygen shares its two unpaired electrons with two separate hydrogen atoms.
- This head-on overlap creates two strong, single covalent bonds called **sigma (σ) bonds**.
- In a water molecule, the oxygen atom is surrounded by four pairs of electrons. If all four pairs were identical, they would spread out evenly into a perfect pyramid shape (tetrahedron) with angles of (109.5^o). However, because two of those pairs are not shared with hydrogen, they take up extra space and squeeze the bonds, so the H-O-H bond angle is (104.5^o).

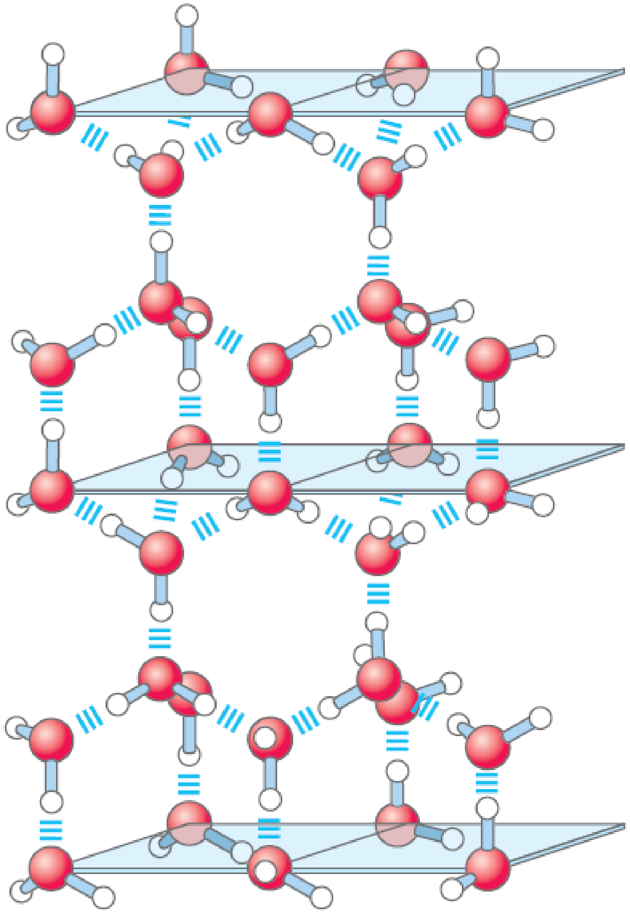
Hydrogen bond

- The oxygen nucleus attracts electrons more strongly than does the hydrogen nucleus (a proton); that is, oxygen is more electronegative.
- The sharing of electrons between H and O is therefore unequal; the electrons are more often in the vicinity of the oxygen atom than of the hydrogen.
- The result of this unequal electron sharing is two electric dipoles in the water molecule, one along each of the H-O bonds; each hydrogen bears a partial positive charge (δ^+) and the oxygen atom bears a partial negative charge equal to the sum of the two partial positives ($2\delta^-$).
- As a result, there is an electrostatic attraction between the oxygen atom of one water molecule and the hydrogen of another, called a **hydrogen bond.**
- Hydrogen bonds are relatively weak. Those in liquid water have a **bond dissociation energy** (the energy required to break a bond) of about 23 kJ/mol, compared with 470 kJ/mol for the covalent O-H bond in water or 348 kJ/mol for a covalent C-C bond.



Hydrogen bond

- At any given time, most of the molecules in liquid water are engaged in hydrogen bonding, but the lifetime of each hydrogen bond is just 1 to 20 picoseconds (1 ps = 10^{12} s); upon breakage of one hydrogen bond, another hydrogen bond forms, with the same partner or a new one, within 0.1 ps.
- The apt phrase “flickering clusters” has been applied to the short-lived groups of water molecules interlinked by hydrogen bonds in liquid water.
- The sum of all the hydrogen bonds between H_2O molecules confers great internal cohesion on liquid water.
- Extended networks of hydrogen-bonded water molecules also form bridges between solutes (proteins and nucleic acids, for example) that allow the larger molecules to interact with each other over distances of several nanometers without physically touching.
- The nearly tetrahedral arrangement of the orbitals about the oxygen atom allows each water molecule to form hydrogen bonds with as many as four neighboring water molecules.
- In liquid water at room temperature and atmospheric pressure, however, water molecules are disorganized and in continuous motion, so that each molecule forms hydrogen bonds with an average of only 3.4 other molecules.
- In ice, on the other hand, each water molecule is fixed in space and forms hydrogen bonds with a full complement of four other water molecules to yield a regular lattice structure.



Water Forms Hydrogen Bonds with Polar Solutes

- Hydrogen bonds are not unique to water.
- They readily form between an electronegative atom (the hydrogen acceptor, usually oxygen or nitrogen with a lone pair of electrons) and a hydrogen atom covalently bonded to another electronegative atom (the hydrogen donor) in the same or another molecule (Fig. 2–3).
- Hydrogen atoms covalently bonded to carbon atoms do not participate in hydrogen bonding, because carbon is only slightly more electronegative than hydrogen and thus the COH bond is only very weakly polar.
- Hydrogen bonds are strongest when the bonded molecules are oriented to maximize electrostatic interaction,which occurs when the hydrogen atom and the two atoms that share it are in a straight line—that is, when the acceptor atom is in line with the covalent bond between the donor atom and H (Fig. 2–5).

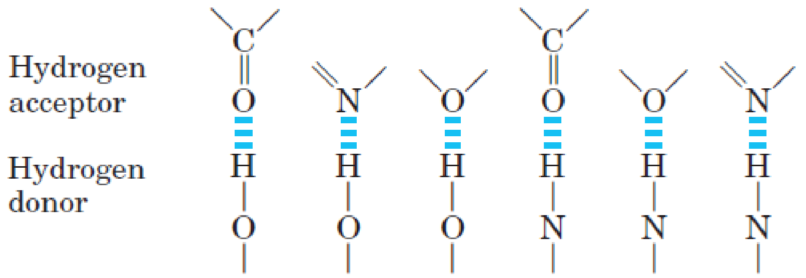


FIGURE 2–3 Common hydrogen bonds in biological systems. The hydrogen acceptor is usually oxygen or nitrogen; the hydrogen donor is another electronegative atom.

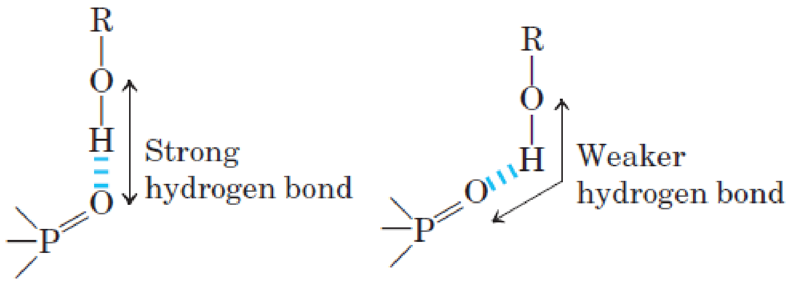


FIGURE 2–5 Directionality of the hydrogen bond. The attraction between the partial electric charges (see Fig. 2–1) is greatest when the three atoms involved (in this case O, H, and O) lie in a straight line. When the hydrogen-bonded moieties are structurally constrained (as when they are parts of a single protein molecule, for example), this ideal geometry may not be possible and the resulting hydrogen bond is weaker.

Water Interacts Electrostatically with Charged Solutes

- Water is a polar solvent. It readily dissolves most biomolecules, which are generally charged or polar compounds (Table 2–2); compounds that dissolve easily in water are **hydrophilic.**
- Water dissolves salts such as NaCl by hydrating and stabilizing the Na and Cl ions, weakening the electrostatic interactions between them and thus counteracting their tendency to associate in a crystalline lattice.
- As a salt such as NaCl dissolves, the Na and Cl ions leaving the crystal lattice acquire far greater freedom of motion (Fig. 2–6).
- The resulting increase in entropy (randomness) of the system is largely responsible for the ease of dissolving salts such as NaCl in water.

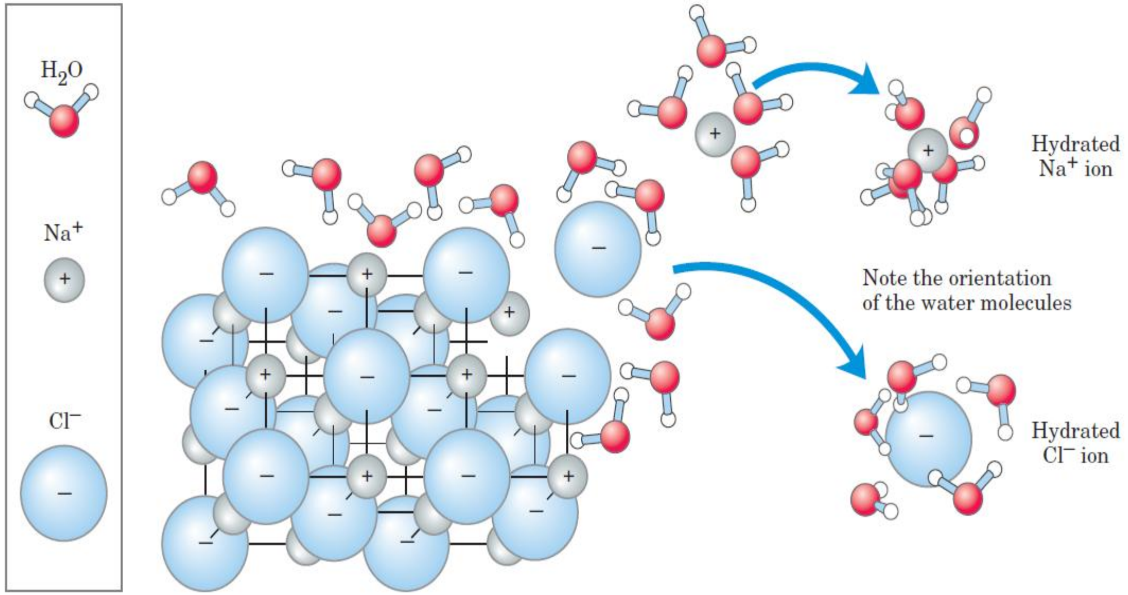
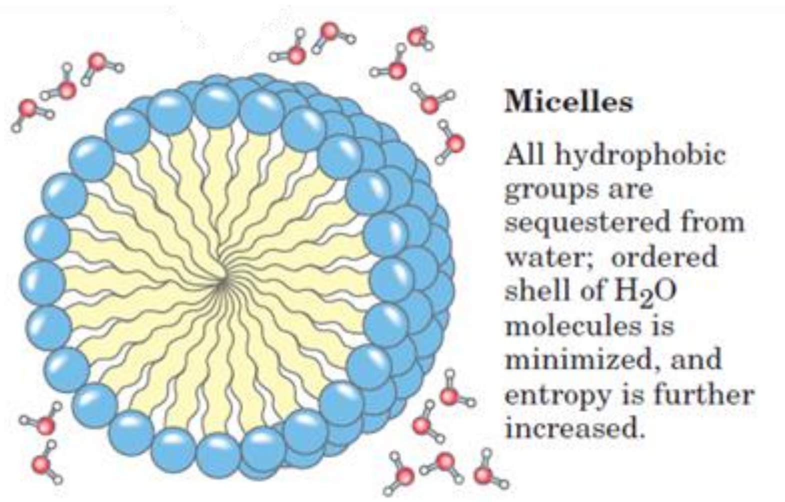


FIGURE 2–6 Water as solvent. Water dissolves many crystalline salts by hydrating their component ions. The NaCl crystal lattice is disrupted as water molecules cluster about the Cl^- and Na^+ ions. The ionic charges are partially neutralized, and the electrostatic attractions necessary for lattice formation are weakened.

Nonpolar Compounds Force Energetically Unfavorable Changes in the Structure of Water

- Nonpolar molecules in aqueous solution interfere with the hydrogen bonding of some water molecules in their immediate vicinity, but polar or chargedsolutes (such as NaCl) compensate for lost water-water hydrogen bonds by forming new solute-water interactions.
- **Amphipathic** compounds contain regions that are polar (or charged) and regions that are nonpolar.
- When an amphipathic compound is mixed with water, the polar, hydrophilic region interacts favorably with the solvent and tends to dissolve, but the nonpolar, hydrophobic region tends to avoid contact with the water.
- The nonpolar regions of the molecules cluster together to present the smallest hydrophobic area to the aqueous solvent, and the polar regions are arranged to maximize their interaction with the solvent.
- These stable structures of amphipathic compounds in water, called **micelles,** may contain hundreds or thousands of molecules.



Osmotic Pressure

- The physical properties of aqueous solutions are strongly influenced by the concentrations of solutes.
- When two aqueous compartments are separated by a semipermeable membrane (such as the plasma membrane separating a cell from its surroundings), water moves across that membrane to equalize the osmolarity in the two compartments.
- This tendency for water to move across a semipermeable membrane is the osmotic pressure.